

# On the spectral radii of bicyclic graphs with fixed independence number

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## Abstract

Bicyclic graph is a connected graph in which the number of edges equals the number of vertices plus one. In this paper, we determine the graph which alone maximizes the spectral radii among all the bicyclic graphs on  $n$  vertices with fixed independence number.

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*Keywords:* Bicyclic graph; Independence number; Spectral radius

## 1 Introduction

Let  $G$  be a simple graph. Denote by  $N_G(v)$  (or simply  $N(v)$ ) the set of all the neighbors of a vertex  $v$  in  $G$ , and by  $d_G(v)$  (or  $d(v)$ ) the degree of  $v$ . Let  $A(G)$  be the adjacency matrix of  $G$  and  $\Phi(G; x)$  be the characteristic polynomial  $\det(xI - A(G))$ . Since  $A(G)$  is a real symmetric matrix, all of its eigenvalues are real. The largest eigenvalue of  $A(G)$  is called the spectral radius of  $G$ , denoted by  $\rho(G)$ . When  $G$  is connected,  $A(G)$  is an irreducible matrix. And by the Perron-Frobenius Theorem  $\rho(G)$  has multiplicity one and there exists a unique unit positive eigenvector corresponding to  $\rho(G)$ . We shall refer to such an eigenvector as the Perron vector of  $G$ . Let  $x$  be the Perron vector of a connected graph  $G$ , and we always use  $x_u$  to denote the coordinate of  $x$  corresponding to the vertex  $u$  of  $G$ .

Brualdi and Solheid [1] proposed the following general problem, which became one of the classic problems of spectral graph theory:

*Given a set of graphs, find an upper bound for the spectral radius and characterize the graphs in which the maximal spectral radius is attained.*

A subset  $S$  of  $V(G)$  is called an independent set of  $G$  if no two vertices in  $S$  are adjacent in  $G$ . The independence number of  $G$ , denoted by  $\alpha(G)$ , is the size of a maximum independent set of  $G$ . We use the notations in [5]. Denote by  $\alpha'(G)$  the edge independence number (or matching number), by  $\beta(G)$  the vertex covering number, and  $\beta'(G)$  the edge covering number for graph  $G$ . For a tree  $T$  on  $n$  vertices  $\alpha(T) = n - \alpha'(T)$  (see Lemmas 2.4, 2.5). In [6] the tree with the maximal spectral radius among all the trees on  $n$  vertices with fixed matching number was determined. Thus the tree with the maximal spectral radius among all the trees on  $n$  vertices with fixed independence number was also determined. In [9] the graph with the maximal spectral radius among all the unicyclic graphs on  $n$  vertices with fixed independence number was determined.

Here we are interested in finding the graph with the maximal spectral radius among all the bicyclic graphs on  $n$  vertices with fixed independence number. We mainly prove the following results.

**Theorem 1.1.** *Let  $F(n, \frac{n-2}{2})$  and  $M(n, \alpha)$  be the graphs as shown in Fig. 2 and Fig. 3. For a bicyclic graph  $G$  on  $n$  ( $n \geq 10$ ) vertices then*

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(1).  $\alpha(G) \geq \frac{n-2}{2}$ ;

(2). if  $\alpha(G) = \frac{n-2}{2}$ , then  $\rho(G) \leq \rho(F(n, \frac{n-2}{2}))$ , where  $\rho(F(n, \frac{n-2}{2}))$  is the largest root of the equation

$$x^4 - 2x^3 - (n/2 + 1)x^2 + nx + 3 = 0,$$

and equality holds if and only if  $G = F(n, \frac{n-2}{2})$ ;

(3). if  $\alpha(G) \geq \frac{n-1}{2}$ , then  $\rho(G) \leq \rho(M(n, \alpha))$ , where  $\rho(M(n, \alpha))$  is the largest root of the equation

$$x^4 - (\alpha + 3)x^2 - 4x + (2\alpha - n + 1) = 0,$$

and equality holds if and only if  $G = M(n, \alpha)$ .

## 2 Preliminaries

The the following two lemmas are the main tools for some proofs in later sections.

**Lemma 2.1.** [10] Let  $u, v$  be two vertices of a connected graph  $G$ . Suppose  $v_1, v_2, \dots, v_s$  ( $1 \leq s \leq d(v)$ ) are some vertices in  $N(v) \setminus (N(u) \cup \{u\})$ . Let  $x$  be the Perron vector of  $G$ . If  $x_u \geq x_v$ , let  $G^*$  be the graph obtained from  $G$  by deleting the edges  $vv_1, vv_2, \dots, vv_s$  and adding the edges  $uv_1, uv_2, \dots, uv_s$ , then we have  $\rho(G^*) > \rho(G)$ .

**Lemma 2.2.** [4] Let  $v$  be a vertex in a non-trivial connected graph  $G$  and suppose that two paths of lengths  $k, m$  ( $k \geq m \geq 1$ ) are attached to  $G$  by their end vertices at  $v$  to form  $G_{k,m}$ . Then  $\rho(G_{k,m}) > \rho(G_{k+1,m-1})$ .

**Lemma 2.3.** [12] For any simple graph  $G$  we have  $\rho(G) \geq \sqrt{\Delta(G)}$  holds.

**Lemma 2.4.** [] Let  $G$  be a graph on  $n$  vertices without isolated vertices. Then

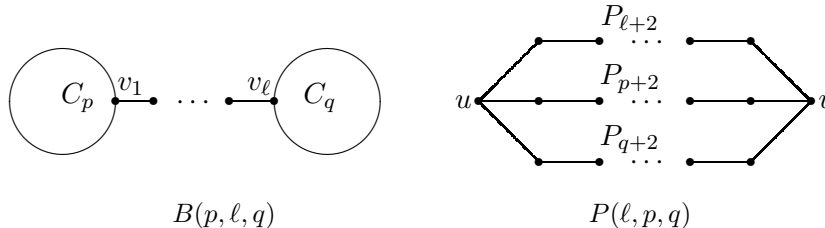
$$\alpha(G) + \beta(G) = \alpha'(G) + \beta'(G) = n.$$

**Lemma 2.5.** [] Let  $G$  be a bipartite graph without isolated vertices. Then  $\alpha(G) = \beta'(G)$ .

**Lemma 2.6.** [3] Let  $v$  be a vertex of  $G$ , and  $\mathcal{C}(v)$  be the set of all cycles containing  $v$ . Then

$$\Phi(G; x) = x\Phi(G - v; x) - \sum_{u \in N(v)} \Phi(G - u - v; x) - 2 \sum_{Z \in \mathcal{C}(v)} \Phi(G - V(Z); x).$$

Let  $C_p$  and  $C_q$  be two vertex-disjoint cycles. Suppose that  $v_1$  is a vertex of  $C_p$  and  $v_\ell$  is a vertex of  $C_q$ . Joining  $v_1$  and  $v_\ell$  by a path  $v_1v_2 \dots v_\ell$  on  $\ell$  vertices, where  $\ell \geq 1$  and  $\ell = 1$  means identifying  $v_1$  with  $v_\ell$ , the resulting graph (see Fig.1), denoted by  $B(p, \ell, q)$ , is called an  $\infty$ -graph. Let  $P_{\ell+2}, P_{p+2}$  and  $P_{q+2}$  be three vertex-disjoint paths, where  $0 \leq \ell \leq p \leq q$  and at most one of them is 0. Identifying the three initial vertices and terminal vertices of them, respectively, the resulting graph (see Fig.1), denoted by  $P(\ell, p, q)$ , is called a  $\theta$ -graph. Obviously  $\mathcal{B}(n)$  consists of two types of graphs: one type, denoted by  $\mathcal{B}_1(n)$ , are those graphs each of which is an  $\infty$ -graph or an  $\infty$ -graph with trees attached; the other type, denoted by  $\mathcal{B}_2(n)$ , are those graphs each of which is a  $\theta$ -graph or a  $\theta$ -graph with trees attached.



**Fig. 1** the graphs  $B(p, \ell, q)$  and  $P(\ell, p, q)$

The base of a bicyclic graph  $G$ , denoted by  $\widehat{G}$ , is the (unique) minimal bicyclic subgraph of  $G$ . We use  $V_c(G)$  to denote all the vertices on the cycles of a graph  $G$ .

**Lemma 2.7.** *Let  $G$  be a graph in  $\mathcal{B}(n)$ . Then*

- (1).  $\alpha(G) \geq \frac{n-2}{2}$ ;
- (2).  $\alpha(G) = \frac{n-2}{2}$  if and only if  $\widehat{G} = B(p, \ell, q)$  for some three integers  $p, \ell, q$ , where  $\ell \geq 2$ ,  $p, q$  are odd, and the graph  $G - V_c(G)$  has a perfect matching.

*Proof.* (1). Let  $G$  be a graph in  $\mathcal{B}(n)$ . Then  $\widehat{G}$  is an  $\infty$ -graph, or a  $\theta$ -graph. When  $\widehat{G} = B(p, \ell, q)$  for some three integers  $p, \ell, q$ , where  $\ell \geq 2$ , and  $p, q$  are odd, let  $v_1$  be a vertex on the cycle  $C_p$ , and  $v_\ell$  be a vertex on the cycle  $C_q$ . Then  $G - v_1 - v_\ell$  is a forest, and so  $\alpha(G) \geq \alpha(G - v_1 - v_\ell) \geq \frac{n-2}{2}$ . For other cases we may always choose a proper vertex of  $G$ , say  $v$ , such that  $G - v$  is a bipartite graph, and then  $\alpha(G) \geq \alpha(G - v) \geq \frac{n-1}{2}$ .

(2). From the proof of (1) we know that if  $\alpha(G) = \frac{n-2}{2}$ , then  $\widehat{G} = B(p, \ell, q)$ , where  $\ell \geq 2$ ,  $p, q$  are odd. Now we prove that the graph  $G - V_c(G)$  has a perfect matching. Let

$$G - V_c(G) = T_1 \bigcup \cdots \bigcup T_s,$$

where  $T_i$  is a tree for each  $i = 1, \dots, s$ . Suppose to the contrary that  $T_1$  has no perfect matching. Write  $|V(T_1)| = t$ , then  $\alpha'(T_1) \leq \frac{t-1}{2}$ . By König-Egverary theorem we have

$$\alpha(T_1) = \beta'(T_1) = t - \alpha'(T_1) \geq \frac{t+1}{2}.$$

Let  $S_1$  be an independent set of  $T_1$  with  $|S_1| = \alpha(T_1)$ . Let  $u$  be the vertex on the cycle and  $u$  has a neighbour in  $T_1$ , and  $v$  be a vertex on another cycle of  $G$ . Then  $G - u - v - V(T_1)$  is a forest. Let  $S_2$  be an independent set of  $G - u - v - V(T_1)$  with  $|S_2| = \alpha(G - u - v - V(T_1)) \geq \frac{n-t-2}{2}$ . The fact that  $u \notin (S_1 \cup S_2)$  insures that  $S_1 \cup S_2$  is an independent set of  $G$ . Thus  $\alpha(G) \geq |S_1 \cup S_2| \geq \frac{n-1}{2}$ . This contradicts the hypothesis that  $\alpha(G) = \frac{n-2}{2}$ .

Now we prove the sufficiency for (2).

Write  $|V_c(G)| = k$ . If  $\widehat{G} = B(p, \ell, q)$ , where  $\ell \geq 2$ ,  $p, q$  are odd, then any independent set of  $G$  contains at most  $\frac{k-2}{2}$  vertices in  $V_c(G)$ . And if the graph  $G - V_c(G)$  has a perfect matching, then any independent set of  $G$  contains at most  $\frac{n-k}{2}$  vertices outside of  $V_c(G)$ . Thus  $\alpha(G) \leq \frac{n-2}{2}$ . And we have proved that  $\alpha(G) \geq \frac{n-2}{2}$ . So  $\alpha(G) = \frac{n-2}{2}$ .  $\square$

Let

$$\mathcal{B}(n, \alpha) = \{G \mid G \in \mathcal{B}(n), \alpha(G) = \alpha\},$$

from Lemma 2.7 we know that  $\alpha \geq \frac{n-2}{2}$ . In Section 3 we will determine the graph with maximal spectral radius in  $\mathcal{B}(n, \frac{n-2}{2})$ . When  $\alpha \geq \frac{n-1}{2}$  the graph with maximal spectral radius in  $\mathcal{B}(n, \alpha)$  will be determined in Section 4.

### 3 The graph with maximal spectral radius in $\mathcal{B}(n, \frac{n-2}{2})$

Let  $F(n, \frac{n-2}{2})$  be the graph as shown in Fig.2. In this section we will prove that  $F(n, \frac{n-2}{2})$  alone maximizes the spectral radius among the graphs in  $\mathcal{B}(n, \frac{n-2}{2})$  when  $n \geq 10$ .

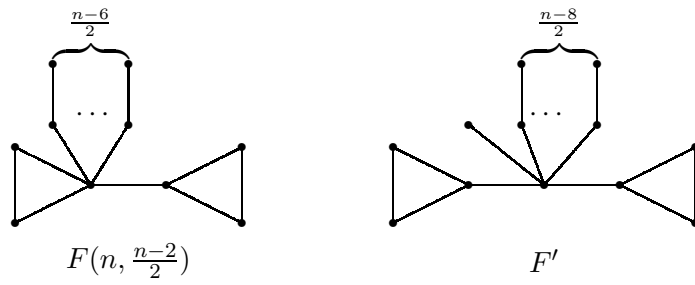


Fig.2 the graphs  $F(n, \frac{n-2}{2})$  and  $F'$

**Lemma 3.1.** *Let  $F'$  and  $F(n, \frac{n-2}{2})$  be the graphs as shown in Fig.2. Then  $\rho(F(n, \frac{n-2}{2})) > \rho(F')$ .*

*Proof.* Write  $n = 2c$ . By using Lemma 2.6 and tedious calculations we have

$$\Phi(F(n, \frac{n-2}{2}); x) = (x^2 - 1)^{c-3}(x+1)^2[x^4 - 2x^3 - (c+1)x^2 + 2cx + 3],$$

$$\Phi(F'; x) = (x^2 - 1)^{c-5}(x+1)^4(x-2)(x^5 - 2x^4 - cx^3 + 2cx^2 - x - 2).$$

Set

$$g(x) = (x-1)^2[x^4 - 2x^3 - (c+1)x^2 + 2cx + 3],$$

and

$$h(x) = (x-2)(x^5 - 2x^4 - cx^3 + 2cx^2 - x - 2),$$

then  $\rho(F(n, \frac{n-2}{2}))$  is the largest root of the equation  $g(x) = 0$ , and  $\rho(F')$  is the largest root of the equation  $h(x) = 0$ . When  $n \geq 10$ , i.e.,  $c \geq 5$  we have  $\rho(F') \geq \sqrt{\Delta(F')} > 2$ , and it may be verified that

$$h(x) - g(x) = (c-3)x(x-2) + 1,$$

then  $g(\rho(F')) < 0$ . Thus the largest root of the equation  $g(x) = 0$  is larger than  $\rho(F')$ , i.e.,  $\rho(F(n, \frac{n-2}{2})) > \rho(F')$ .  $\square$

**Theorem 3.1.** *Graph  $F(n, \frac{n-2}{2})$  alone maximizes the spectral radius among the graphs in  $\mathcal{B}(n, \frac{n-2}{2})$  when  $n \geq 10$ .*

*Proof.* Suppose  $G^*$  is a graph with maximal spectral radius among the graphs in  $\mathcal{B}(n, \frac{n-2}{2})$ . From (2) of Lemma 2.7 we know that  $\widehat{G^*} = B(p, \ell, q)$  for some three integers  $p, \ell, q$ , where  $\ell \geq 2$ ,  $p, q$  are odd, and the subgraph  $G^* - V_c(G^*)$  has a perfect matching. Denote by  $v_1 v_2 \cdots v_{\ell-1} v_\ell$  the path joining the cycles  $C_p$  and  $C_q$ , where  $v_1$  lies on  $C_p$  and  $v_\ell$  lies on  $C_q$ . Let  $x$  be the Perron vector of  $G^*$ .

**Claim 1.** Any vertex in  $V_c(G^*) \setminus \{v_1, v_\ell\}$  has degree 2.

**Proof of Claim 1.** Suppose to the contrary that there exists a vertex in  $V_c(G^*) \setminus \{v_1, v_\ell\}$ , say  $w$ , with degree at least 3. Without loss of generality assume that  $w$  lies on  $C_p$ . Let  $w'$  be a neighbour of  $w$  such that  $w' \notin V_c(G^*)$ . Set

$$G' = \begin{cases} G^* - ww' + v_1 w', & \text{if } x_{v_1} \geq x_w; \\ G^* - v_1 v_2 + w v_2, & \text{if } x_w > x_{v_1}. \end{cases}$$

Then  $G' - V_c(G')$  also has a perfect matching, furthermore  $G'$  is in  $\mathcal{B}(n, \frac{n-2}{2})$ . While we have  $\rho(G') > \rho(G^*)$  from Lemma 2.1. This contradicts the definition of  $G^*$ .

**Claim 2.**  $p = q = 3$ .

**Proof of Claim 2.** Suppose to the contrary that  $p \geq 5$ . Denote by  $C_p = v_1 w_1 w_2 \cdots w_{p-1} w_p (= v_1)$ .

Set

$$G' = \begin{cases} G^* - w_{p-1} v_1 + w_2 v_1, & \text{if } x_{w_2} \geq x_{w_{p-1}}; \\ G^* - w_2 w_1 + w_{p-1} w_1, & \text{if } x_{w_{p-1}} > x_{w_2}. \end{cases}$$

Then  $G'$  is also in  $\mathcal{B}(n, \frac{n-2}{2})$ , while  $\rho(G') > \rho(G^*)$ .

By comparing the coordinates  $x_{v_1}$  and  $x_{v_\ell}$  and using Lemma 2.1, we may prove that at most one of  $\{v_1, v_\ell\}$  with degree more than 3. Next we may suppose that  $d(v_1) \geq d(v_\ell)$ .

**Claim 3.** At most one vertex outside of  $V_c(G^*)$  has degree more than 3.

**Proof of Claim 3.** Suppose to the contrary that there exist two vertices, say  $u, v$ , outside of  $V_c(G^*)$  with degree more than 3. Without loss of generality assume that  $x_u \geq x_v$ . Let  $v'$  be a neighbour of  $v$  on the path between  $u$  and  $v$ ,  $v''$  be the vertex saturated by  $v$  in a perfect matching of  $G^* - V_c(G^*)$ . Since  $d(v) \geq 3$ , we may suppose that  $w \in (N(v) \setminus \{v', v''\})$ . Set  $G' = G^* - vw + uw$ . Then  $G'$  is also in  $\mathcal{B}(n, \frac{n-2}{2})$ , while  $\rho(G') > \rho(G^*)$ .

By using the similar arguments as the proof of Claim 3, we may prove that if  $d(v_1) \geq 4$  then each vertex outside of  $V_c(G^*)$  has degree at most 2.

**Claim 4.**  $\ell \leq 3$ .

**Proof of Claim 4.** Suppose to the contrary that  $\ell \geq 4$ , then  $v_2 \neq v_{\ell-1}$ . Set

$$G' = \begin{cases} G^* - v_{\ell-1}v_\ell + v_2v_\ell, & \text{if } x_{v_2} \geq x_{v_{\ell-1}}; \\ G^* - v_2v_1 + v_{\ell-1}v_1, & \text{if } x_{v_{\ell-1}} > x_{v_2}. \end{cases}$$

Then  $G'$  is also in  $\mathcal{B}(n, \frac{n-2}{2})$ , while  $\rho(G') > \rho(G^*)$ . Thus  $\ell \leq 3$ .

Furthermore by using the above results and Lemma 2.2 we have if  $\ell = 2$ , then  $G^* = F(n, \frac{n-2}{2})$ . If  $\ell = 3$ , then  $G^* = F'$ , while from Lemma 3.1 we know that  $\rho(F') < \rho(F(n, \frac{n-2}{2}))$ . Thus  $\ell = 2$  and we have  $G^* = F(n, \frac{n-2}{2})$ .  $\square$

## 4 The graph with maximal spectral radius in $\mathcal{B}(n, \alpha)$ when $\alpha \geq \frac{n-1}{2}$

It is easy to see that every connected graph  $G$  has at most  $\alpha(G)$  pendant vertices. In this section we may suppose  $\alpha \geq \frac{n-1}{2}$ . Now we give a partition for the graphs in  $\mathcal{B}(n, \alpha)$  according to the number of the pendant vertices.

Class (C1): The graphs in  $\mathcal{B}(n, \alpha)$  with  $k$  pendant vertices, where  $k \leq \alpha - 2$ .

Class (C2): The graphs in  $\mathcal{B}(n, \alpha)$  with  $\alpha - 1$  pendant vertices.

Class (C3): The graphs in  $\mathcal{B}(n, \alpha)$  with  $\alpha$  pendant vertices.

We will discuss the spectral radii of the graphs in Class (C1) in Section 4.1, the spectral radii of the graphs in Class (C3) in Section 4.2, and the spectral radii of the graphs in Class (C2) in Section 4.3.

### 4.1 The graphs in $\mathcal{B}(n, \alpha)$ with $k$ pendant vertices and $k \leq \alpha - 2$ .

Let  $B^\sharp(k)$  be the graph on  $n$  vertices, obtained by attaching  $k$  paths of almost equal length to the vertex with degree 4 of  $B(3, 1, 3)$ . The following result was shown in [7] and

**Lemma 4.1.** ([7, ?]) Suppose  $G$  is a bicyclic graph on  $n$  vertices with  $k$  pendant vertices, then  $\rho(G) \leq \rho(B^\sharp(k))$ , with equality if and only if  $G = B^\sharp(k)$ .

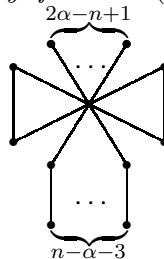


Fig.3 the graph  $M(n, \alpha)$

**Theorem 4.1.** Let  $G$  be a graph in  $\mathcal{B}(n, \alpha)$  with  $k$  pendant vertices. When  $k \leq \alpha - 2$  and  $\alpha \geq \frac{n-2}{2}$ , we have  $\rho(G) \leq \rho(M(n, \alpha))$  with equality if and only if  $G = M(n, \alpha)$ .

*Proof.* First by using Lemma 2.2 directly we have if  $1 \leq k \leq n - 6$ , then  $\rho(B^\sharp(k)) < \rho(B^\sharp(k + 1))$ . It is easy to see that when  $\alpha \geq \frac{n-1}{2}$ , then  $B^\sharp(\alpha - 2) = M(n, \alpha)$ . Then from Lemma 4.1 we have

$$\rho(G) \leq \rho(B^\sharp(k)) \leq \rho(B^\sharp(\alpha - 2)) = \rho(M(n, \alpha)).$$

Furthermore it is not difficult to see that the quality holds if and only if  $G = M(n, \alpha)$ .  $\square$

## 4.2 The graphs in $\mathcal{B}(n, \alpha)$ with $\alpha$ pendant vertices

Set

$$\mathcal{B}(n, \alpha, \alpha) = \{G \mid G \in \mathcal{B}(n, \alpha) \text{ and } G \text{ contains } \alpha \text{ pendant vertices}\}.$$

In this section we will prove that the spectral radii of the graphs in  $\mathcal{B}(n, \alpha, \alpha)$  are less than that of  $M(n, \alpha)$ . It is easy to see that a graph  $G$  is in  $\mathcal{B}(n, \alpha, \alpha)$  if and only if  $G \in \mathcal{B}(n, \alpha)$  and every non-pendant vertex of  $G$  has at least one pendant neighbour. For  $i = 1, 2$  set

$$\mathcal{B}_i(n, \alpha, \alpha) = \{G \mid G \in \mathcal{B}(n, \alpha, \alpha) \text{ and } G \in \mathcal{B}_i(n)\}.$$

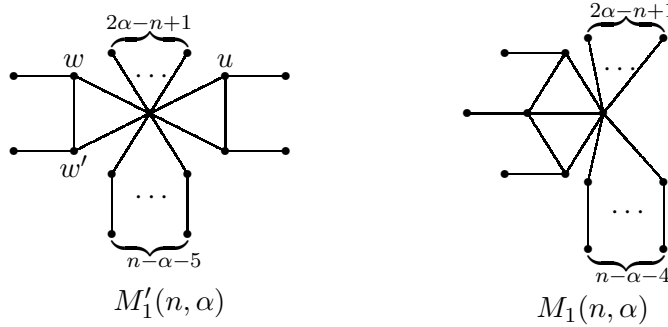


Fig. 4 the graphs  $M'_1(n, \alpha)$  and  $M_1(n, \alpha)$

**Lemma 4.2.** Let  $M_1(n, \alpha)$  and  $M(n, \alpha)$  be the graphs as shown in Fig. 3 and Fig. 4. Then  $\rho(M_1(n, \alpha)) < \rho(M(n, \alpha))$ .

*Proof.* Let

$$f(x) = x^4 - (\alpha + 3)x^2 - 4x + (2\alpha - n + 1). \quad (1)$$

By using Lemma 2.6 and tedious calculations we have

$$\Phi(M(n, \alpha); x) = x^{2\alpha-n}(x^2 - 1)^{n-\alpha-2}f(x), \quad (2)$$

and  $\rho(M(n, \alpha))$  is the largest root of the equation  $f(x) = 0$ . Let

$$f_1(x) = x^8 - (\alpha + 5)x^6 - 4x^5 - (n - 6\alpha)x^4 + 4x^3 + (4n - 9\alpha - 5)x^2 - 2x - (n - 2\alpha - 1).$$

We have

$$\Phi(M_1(n, \alpha); x) = x^{2\alpha-n}(x^2 - 1)^{n-\alpha-4}f_1(x),$$

and  $\rho(M_1(n, \alpha))$  is the largest root of the equation  $f_1(x) = 0$ . It may be verified that

$$f_1(x) - (x^2 - 1)^2 f(x) = 2x[(\alpha - 4)x^3 - 2x^2 + (n - 2\alpha)x + 2]. \quad (3)$$

For  $M_1(n, \alpha)$  when  $n \geq 10$  we have  $\alpha \geq 5$ , and write  $\rho(M_1(n, \alpha)) = \rho$ , then  $\rho > 2$ . Then from (3) we have

$$\begin{aligned} -\frac{(\rho^2 - 1)^2}{2\rho} f(\rho) &= (\alpha - 4)\rho^3 - 2\rho^2 + (n - 2\alpha)\rho + 2 \\ &> (2\alpha - 10)\rho^2 + (n - 2\alpha)\rho + 2 \\ &> (n + 2\alpha - 20)\rho + 2 > 0. \end{aligned}$$

Thus  $f(\rho) < 0$ , then the largest root of equation  $f(x) = 0$  is larger than  $\rho$ , i.e.,  $\rho(M(n, \alpha)) > \rho(M_1(n, \alpha))$ .  $\square$

**Lemma 4.3.** *Graph  $M'_1(n, \alpha)$  alone maximizes the spectral radius among all the graphs in  $\mathcal{B}_1(n, \alpha, \alpha)$ .*

*Proof.* Suppose  $G^*$  is a graph with maximal spectral radius among the graphs in  $\mathcal{B}_1(n, \alpha, \alpha)$ . Write  $\widehat{G^*} = B(p, \ell, q)$ . Let  $x$  be the Perron vector of  $G^*$ . Now we will prove some properties for  $G^*$ .

**Claim 1.**  $\ell = 1$ .

**Proof of Claim 1.** Suppose to the contrary that  $\ell \geq 2$ , and  $v_1, v_\ell$  are the vertices of  $G^*$  with  $d_{\widehat{G^*}}(v_1) = d_{\widehat{G^*}}(v_\ell) = 3$ . Without loss of generality assume that  $x_{v_1} \geq x_{v_\ell}$ . Set

$$N(v_\ell) = \{v'_\ell, v''_\ell, v_{\ell 1}, \dots, v_{\ell s}\},$$

where  $d(v'_\ell) = 1$ , and  $v''_\ell$  is the neighbour of  $v_\ell$  lying on the path between  $v_1$  and  $v_\ell$ . Then  $s \geq 2$  follows from the fact that  $d_{G^*}(v_\ell) \geq 4$ . Set

$$G' = G^* - v_\ell v_{\ell 1} - \dots - v_\ell v_{\ell s} + v_1 v_{\ell 1} + \dots + v_1 v_{\ell s}.$$

Then  $G'$  is in  $\mathcal{B}_1(n)$  with  $\alpha$  pendant vertices, and every non-pendant vertex of  $G'$  has at least one pendant neighbour. Thus  $G'$  is also in  $\mathcal{B}_1(n, \alpha, \alpha)$ . While we have  $\rho(G') > \rho(G^*)$ . This contradicts the definition of  $G^*$ .

**Claim 2.**  $p = q = 3$ .

**Proof of Claim 2.** Suppose to the contrary that  $p \geq 4$ , and  $uv$  is an edge of the cycle  $C_p$ . Without loss of generality assume that  $x_u \geq x_v$ . Let  $w$  ( $w \neq u$ ) be the neighbour of  $v$  on the cycle  $C_p$ , then  $wu \notin E(G^*)$ . Set  $G' = G^* - vw + uw$ . Then  $G'$  is also in  $\mathcal{B}_1(n, \alpha, \alpha)$ , while  $\rho(G') > \rho(G^*)$ .

Thus from Claim 1 and Claim 2 we have  $\widehat{G^*} = B(3, 1, 3)$ . Denote by  $v$  the vertex of  $G^*$  with  $d_{\widehat{G^*}}(v) = 4$ .

**Claim 3.** Every vertex outside of  $V_c(G^*)$  has degree at most 2.

**Proof of Claim 3.** Suppose to the contrary that there exists a vertex, say  $w$ , such that  $w \notin V_c(G^*)$  with  $d_{G^*}(w) \geq 3$ . Let  $w'$  be a non-pendant neighbour of  $w$ , which does not lie on any path between  $v$  and  $w$ . Let  $v', v''$  be two neighbours of  $v$  on some cycle of  $G^*$ , and  $v', v''$  do not lie on any path between  $v$  and  $w$ . Set

$$G' = \begin{cases} G^* - vv' - vv'' + ww' + ww'', & \text{if } x_w \geq x_v; \\ G^* - ww' + vv', & \text{if } x_v > x_w. \end{cases}$$

Then we obtain a graph also in  $\mathcal{B}_1(n, \alpha, \alpha)$  with larger spectral radius than that of  $G^*$ .

By using the similar arguments as the proof of Claim 3 we may deduce that every vertex in  $V_c(G^*) \setminus \{v\}$  has degree 3. Thus combining the above results we have  $G^* = M'_1(n, \alpha)$ .  $\square$

By using the similar proof as that of Lemma 4.3, we may obtain the following result.

**Lemma 4.4.** *Graph  $M_1(n, \alpha)$  alone maximizes the spectral radius among all the graphs in  $\mathcal{B}_2(n, \alpha, \alpha)$ .*

**Theorem 4.2.** *Let  $G$  be any graph in  $\mathcal{B}(n, \alpha, \alpha)$ . Then  $\rho(G) < \rho(M(n, \alpha))$ .*

*Proof.* Let  $x$  be the Perron vector of  $M'_1(n, \alpha)$ , by symmetry we have  $x_w = x_u$ , where  $u, v$  are shown in Fig.4. It is easy to see that  $M_1(n, \alpha) = M'_1(n, \alpha) - ww' + uw'$ . Then  $\rho(M_1(n, \alpha)) > \rho(M'_1(n, \alpha))$  follows from Lemma 2.1. Let  $G$  be any graph in  $\mathcal{B}(n, \alpha, \alpha)$ . Then by using Lemmas 4.3, 4.4 and 4.2 we have

$$\rho(G) \leq \max\{\rho(M'_1(n, \alpha), \rho(M_1(n, \alpha))\} = \rho(M_1(n, \alpha)) < \rho(M(n, \alpha)).$$

Thus we have  $\rho(G) < \rho(M(n, \alpha))$  for any graph  $G$  in  $\mathcal{B}(n, \alpha, \alpha)$ .  $\square$

### 4.3 The graphs in $\mathcal{B}(n, \alpha)$ with $\alpha - 1$ pendant vertices

Set

$$\mathcal{B}(n, \alpha, \alpha - 1) = \{G \mid G \in \mathcal{B}(n, \alpha) \text{ and } G \text{ contains } \alpha - 1 \text{ pendant vertices}\}.$$

In this section we will prove that the spectral radii of the graphs in  $\mathcal{B}(n, \alpha, \alpha - 1)$  are also less than that of  $M(n, \alpha)$ . For a graph  $G$  in  $\mathcal{B}(n, \alpha, \alpha - 1)$  set

$$V'(G) = \{v \in V(G) \mid d(v) \geq 2 \text{ and } v \text{ has no pendant neighbour}\},$$

then  $|V'(G)| \geq 1$ . Furthermore  $|V'(G)| \leq 3$ , for otherwise  $\alpha - 1$  pendant vertices along with two proper vertices in  $V'(G)$  may form an independent set of  $G$  with cardinality  $\alpha + 1$ . Similarly if  $|V'(G)| = 2$ , then the two vertices in  $V'(G)$  are incident. And if  $|V'(G)| = 3$ , then the vertices in  $V'(G)$  lie on a triangle.

**Lemma 4.5.** *Let  $G^*$  be a graph in  $\mathcal{B}(n, \alpha, \alpha - 1)$  with maximal spectral radius. Then  $|V'(G^*)| \geq 2$ , or  $\rho(G^*) < \rho(M(n, \alpha))$ .*

*Proof.* If  $|V'(G^*)| \geq 2$ , the proof is completed. Now suppose to the contrary that  $|V'(G^*)| = 1$ . Let  $u$  be the vertex in  $V'(G^*)$ , and  $v, w$  are two neighbour of  $u$ . Let  $x$  be the Perron vector of  $G^*$ . Without loss of generality assume that  $x_v \geq x_w$ . Let  $w_1, \dots, w_s$  ( $s \geq 1$ ) be all the pendant neighbours of  $w$ . Set

$$G' = G^* - ww_1 - \dots - ww_s + uw_1 + \dots + uw_s.$$

If  $d_{G'}(w) = 1$ , then every non-pendant vertex of  $G'$  has at least one pendant neighbour, thus  $G' \in \mathcal{B}(n, \alpha, \alpha)$ , and

$$\rho(G^*) < \rho(G') \leq \rho(M(n, \alpha)).$$

If  $d_{G'}(w) \geq 2$ , then  $G'$  is also in  $\mathcal{B}(n, \alpha, \alpha - 1)$ . While  $\rho(G') > \rho(G^*)$ . This contradicts the definition of  $G^*$ .  $\square$

**Lemma 4.6.** *Let  $G$  be a graph in  $\mathcal{B}(n, \alpha, \alpha - 1)$ . If  $|V'(G)| = 2$  and the vertices in  $V'(G)$  do not lie on a triangle, then  $\rho(G) < \rho(M(n, \alpha))$ .*

*Proof.* Suppose  $u, v$  are the two vertices in  $V'(G)$ . Let  $x$  be the Perron vector of  $G$ . Without loss of generality assume that  $x_u \geq x_v$ . Let  $v_1, \dots, v_s$  ( $s \geq 1$ ) be all the neighbours of  $v$  different from  $u$ , then  $v_i \notin N(u)$ . Set

$$G' = G - vv_1 - \dots - vv_s + uv_1 + \dots + uv_s.$$

Then every non-pendant vertex of  $G'$  has at least one pendant neighbour, thus  $G' \in \mathcal{B}(n, \alpha, \alpha)$ . While from Lemma 2.1 and Theorem 4.2 we have  $\rho(G) < \rho(G') \leq \rho(M(n, \alpha))$ .  $\square$



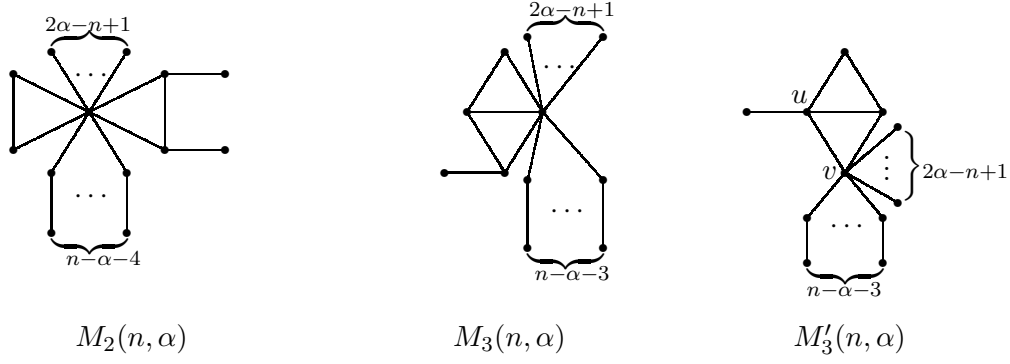


Fig.5 the graphs  $M_2(n, \alpha)$ ,  $M_3(n, \alpha)$  and  $M'_3(n, \alpha)$

**Lemma 4.7.** Let  $M_2(n, \alpha)$  and  $M_3(n, \alpha)$  be the graphs as shown in Fig. 5. Then

- (1).  $\rho(M_2(n, \alpha)) < \rho(M(n, \alpha))$ ;
- (2).  $\rho(M_3(n, \alpha)) < \rho(M(n, \alpha))$ .

*Proof.* Recall that  $\rho(M(n, \alpha))$  is the largest root of the equation  $f(x) = 0$ , where

$$f(x) = x^4 - (\alpha + 3)x^2 - 4x + (2\alpha - n + 1).$$

(1). Let

$$f_2(x) = x^6 - x^5 - (\alpha + 3)x^4 + (\alpha - 2)x^3 - (n - 3\alpha - 5)x^2 + (n - 2\alpha + 1)x - (n - 2\alpha - 1).$$

Then we have

$$\Phi(M_2(n, \alpha); x) = x^{2\alpha-n}(x^2 - 1)^{n-\alpha-4}(x^2 + x - 1)f_2(x).$$

Thus  $\rho(M_2(n, \alpha))$  is the largest root of the equation  $f_2(x) = 0$ , and it can be verified that

$$(x^2 + x - 1)f_2(x) - (x^2 - 1)^2 f(x) = x[(\alpha - 2)x^3 + (n - 2\alpha)x + 2]. \quad (4)$$

For  $M_2(n, \alpha)$  when  $n \geq 10$  we have  $\alpha \geq 5$ , and write  $\rho(M_2(n, \alpha)) = \rho$ , then  $\rho^2 > \Delta(M_2(n, \alpha)) = \alpha + 1$ , and  $\rho > 2$ . Then from (4) we have

$$\begin{aligned} -\frac{(\rho^2 - 1)^2}{\rho} f(\rho) &= (\alpha - 2)\rho^3 + (n - 2\alpha)\rho + 2 \\ &> (\alpha - 2)(\alpha + 1)\rho + (n - 2\alpha)\rho + 2 \\ &= [\alpha(\alpha - 3) + (n - 2)]\rho + 2 > 0. \end{aligned}$$

Thus  $f(\rho) < 0$ , then the largest root of equation  $f(x) = 0$  is larger than  $\rho$ , i.e.,  $\rho(M(n, \alpha)) > \rho(M_2(n, \alpha))$ .

(2). Let

$$f_3(x) = x^8 - (\alpha + 5)x^6 - 4x^5 - (n - 5\alpha - 4)x^4 + 6x^3 + (3n - 7\alpha - 4)x^2 - 2x - (n - 2\alpha - 1),$$

then

$$\Phi(M_3(n, \alpha); x) = x^{2\alpha-n}(x^2 - 1)^{n-\alpha-4}f_3(x).$$

So  $\rho(M_3(n, \alpha))$  is the largest root of the equation  $f_3(x) = 0$ , and it may be verified that

$$f_3(x) - (x^2 - 1)^2 f(x) = x[(\alpha - 4)x^3 - 2x^2 + (n - 2\alpha + 1)x + 2]. \quad (5)$$

For  $M_3(n, \alpha)$  when  $n \geq 10$  we have  $\alpha \geq 5$ , and write  $\rho(M_3(n, \alpha)) = \rho$ , then  $\rho^2 > \Delta(M_3(n, \alpha)) = \alpha + 1$ . Then from (5) we have

$$\begin{aligned}
-\frac{(\rho^2 - 1)^2}{\rho} f(\rho) &= (\alpha - 4)\rho^3 - 2\rho^2 + (n - 2\alpha + 1)\rho + 2 \\
&= (\rho^3 - 2\rho^2 + (\alpha - 5)\rho^3 + (n - 2\alpha + 1)\rho + 2 \\
&> (\rho - 2)(\alpha + 1) + (\alpha - 5)(\alpha + 1)\rho + (n - 2\alpha + 1)\rho + 2 \\
&= (\alpha^2 - 5\alpha + n - 3)\rho - 2\alpha \\
&> 2\alpha(\alpha - 6) + 2n - 6 > 0.
\end{aligned}$$

Thus  $f(\rho) < 0$ , then the largest root of equation  $f(x) = 0$  is larger than  $\rho$ , i.e.,  $\rho(M(n, \alpha)) > \rho(M_3(n, \alpha))$ .  $\square$

Denote by  $\mathcal{B}(n, \alpha, \alpha - 1, 2)$  the set of the graphs  $G$  in  $\mathcal{B}(n, \alpha, \alpha - 1)$  with  $|V'(G)| = 2$  and the vertices in  $V'(G)$  lie on a triangle.

**Lemma 4.8.** *Let  $G$  be a graph in  $\mathcal{B}(n, \alpha, \alpha - 1, 2)$ . Then  $\rho(G) < \rho(M(n, \alpha))$ .*

*Proof.* Let  $G^*$  be a graph with maximal spectral radius in  $\mathcal{B}(n, \alpha, \alpha - 1, 2)$ . First suppose that  $G^*$  is in  $\mathcal{B}_1(n)$ . Then  $\widehat{G^*} = B(3, \ell, q)$ . Let  $u, w$  be the two vertices in  $V'(G^*)$ . By considering some (proper) coordinates of the Perron vector of  $G^*$  and using Lemma 2.1 we may deduce that  $d_{\widehat{G^*}}(u) = d_{\widehat{G^*}}(w) = 2$ . And by using the similar arguments as the proof of Lemma 4.3 we have  $\ell = 1$  and  $q = 3$ . Let  $v$  be the vertex of  $G^*$  with  $d_{\widehat{G^*}}(v) = 4$ . Furthermore we have every vertex outside of  $V_c(G^*)$  has degree at most 2, and the vertex in  $V_c(G^*) \setminus \{u, v, w\}$  has degree 3, and  $d_{G^*}(u) = d_{G^*}(v) = 2$ . Thus we have  $G^* = M_2(n, \alpha)$ . From Lemma 4.7 we know that  $\rho(G^*) < \rho(M(n, \alpha))$ .

Now suppose that  $G^*$  is in  $\mathcal{B}_2(n)$ . Then  $\widehat{G^*} = P(0, 1, q)$ . Similarly as above we may deduce that one vertex in  $V'(G^*)$  has degree 2 in  $\widehat{G^*}$ . Furthermore we have  $G^* \in \{M'_3(n, \alpha), M_3(n, \alpha)\}$ . Considering the coordinates  $x_u$  and  $x_v$  of the Perron vector  $x$  of  $M'_3(n, \alpha)$  and using Lemma 2.1 we may deduce that  $\rho(M'_3(n, \alpha)) < \max\{\rho(M_3(n, \alpha))\}$ . Combining Lemma 4.7 we have

$$\rho(G) \leq \rho(G^*) = \max\{\rho(M'_3(n, \alpha)), \rho(M_3(n, \alpha))\} = \rho(M_3(n, \alpha)) < \rho(M(n, \alpha)).$$

Thus we have  $\rho(G) < \rho(M(n, \alpha))$  for any graph  $G$  in  $\mathcal{B}(n, \alpha, \alpha - 1, 2)$ .  $\square$

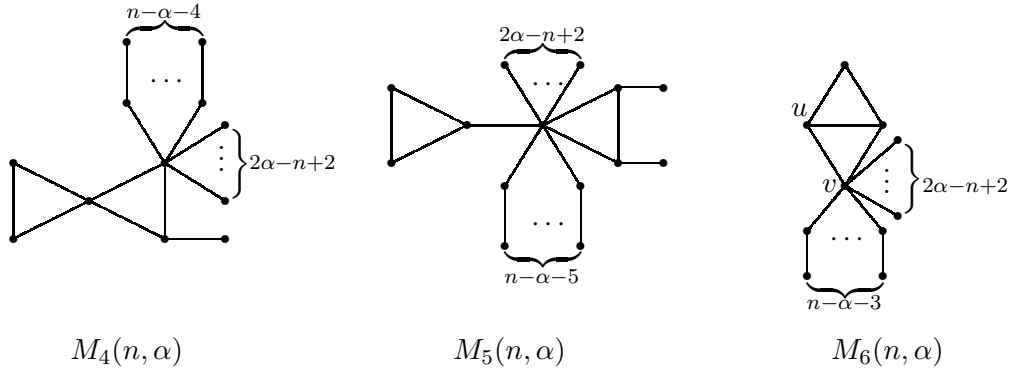


Fig.6 the graphs  $M_4(n, \alpha)$ ,  $M_5(n, \alpha)$  and  $M_6(n, \alpha)$

**Lemma 4.9.** *Let  $M_i(n, \alpha)$  be the graph as shown in Fig.6. Then we have  $\rho(M_i(n, \alpha)) < \rho(M(n, \alpha))$  for each  $i = 4, 5, 6$ .*

*Proof.* Recall that  $\rho(M(n, \alpha))$  is the largest root of the equation  $f(x) = 0$ , where

$$f(x) = x^4 - (\alpha + 3)x^2 - 4x + (2\alpha - n + 1).$$

(1). Let

$$f_4(x) = x^7 - (\alpha + 5)x^5 - 4x^4 - (n - 6\alpha - 3)x^3 + 2(\alpha + 1)x^2 + (4n - 8\alpha - 9)x + 2(n - 2\alpha - 2),$$

then

$$\Phi(M_4(n, \alpha); x) = x^{2\alpha-n+1}(x^2 - 1)^{n-\alpha-4}f_4(x),$$

and  $\rho(M_4(n, \alpha))$  is the largest root of the equation  $f_4(x) = 0$ . And it may be verified that

$$xf_4(x) - (x^2 - 1)^2f(x) = (2\alpha - 5)x^4 + 2(\alpha - 3)x^3 + (2n - 3\alpha - 4)x^2 + 2(n - 2\alpha)x + (n - 2\alpha - 1). \quad (6)$$

For  $M_4(n, \alpha)$  when  $n \geq 10$  we have  $\alpha \geq 5$ , and write  $\rho(M_4(n, \alpha)) = \rho$ , then  $\rho^2 > \Delta(M_3(n, \alpha)) = \alpha$ . Then from (6) we have

$$\begin{aligned} -(\rho^2 - 1)^2f(\rho) &= (2\alpha - 5)\rho^4 + (2\alpha - 6)\rho^3 + (2n - 3\alpha - 4)\rho^2 + (2n - 4\alpha)\rho + (n - 2\alpha - 1) \\ &> [(2\alpha - 5)\alpha + (2n - 3\alpha - 4)]\rho^2 + [(2\alpha - 6)\alpha + (2n - 4\alpha)]\rho + (n - 2\alpha - 1) \\ &> (2\alpha - 5)\alpha + (2n - 3\alpha - 4) + (n - 2\alpha - 1) \\ &= 2\alpha^2 - 10\alpha + 3n - 5 > 0. \end{aligned}$$

Thus  $f(\rho) < 0$ , then the largest root of equation  $f(x) = 0$  is larger than  $\rho$ , i.e.,  $\rho(M(n, \alpha)) > \rho(M_4(n, \alpha))$ .

(2). Let

$$f_5(x) = x^7 - 3x^6 - \alpha x^5 + 3(\alpha + 1)x^4 - (n - \alpha - 4)x^3 + (3n - 8\alpha - 7)x^2 - (n - 2\alpha - 3)x - 2(n - 2\alpha - 2),$$

then we have

$$\Phi(M_5(n, \alpha); x) = x^{2\alpha-n+1}(x^2 - 1)^{n-\alpha-6}(x + 1)^2(x^2 + x + 1)f_5(x).$$

Thus  $\rho(M_5(n, \alpha))$  is the largest root of the equation  $f_5(x) = 0$ , and it may be verified that

$$\begin{aligned} x(x^2 + x + 1)f_5(x) - (x + 1)^2(x^2 - 1)^2f(x) \\ = (2\alpha - 4)x^6 - (2\alpha - 6)x^5 + (2n - 6\alpha + 5)x^4 - (2n - 4\alpha)x^3 - (2n - 5\alpha + 3)x^2 + 2x + (n - 2\alpha - 1). \end{aligned}$$

For  $M_5(n, \alpha)$  when  $n \geq 10$  we have  $\alpha \geq 5$ , and write  $\rho(M_5(n, \alpha)) = \rho$ , then  $\rho > 2$ . Then from (7) we have

$$\begin{aligned} &-(\rho + 1)^2(\rho^2 - 1)^2f(\rho) \\ &= (2\alpha - 4)\rho^6 - (2\alpha - 6)\rho^5 + (2n - 6\alpha + 5)\rho^4 - (2n - 4\alpha)\rho^3 - (2n - 5\alpha + 3)\rho^2 + 2\rho + (n - 2\alpha - 1) \\ &> (2\alpha - 2)\rho^5 + (2n - 6\alpha + 5)\rho^4 - (2n - 4\alpha)\rho^3 - (2n - 5\alpha + 3)\rho^2 + 2\rho + (n - 2\alpha - 1) \\ &> (2n - 2\alpha + 1)\rho^4 - (2n - 4\alpha)\rho^3 - (2n - 5\alpha + 3)\rho^2 + 2\rho + (n - 2\alpha - 1) \\ &> (2n + 2)\rho^3 - (2n - 5\alpha + 3)\rho^2 + 2\rho + (n - 2\alpha - 1) \\ &> (2n + 5\alpha + 1)\rho^2 + 2\rho + (n - 2\alpha - 1) > 0. \end{aligned}$$

Thus  $f(\rho) < 0$ , then the largest root of equation  $f(x) = 0$  is larger than  $\rho$ , i.e.,  $\rho(M(n, \alpha)) > \rho(M_5(n, \alpha))$ .

(3). Let

$$f_6(x) = x^5 - 2x^4 - (\alpha + 2)x^3 + 2(\alpha + 1)x^2 - (n - 2\alpha - 2)x + (2n - 4\alpha - 4),$$

then we have

$$\Phi(M_6(n, \alpha); x) = x^{2\alpha-n+1}(x^2 - 1)^{n-\alpha-4}(x + 1)^2 f_6(x),$$

and  $\rho(M_6(n, \alpha))$  is the largest root of the equation  $f_6(x) = 0$ . And it may be verified that

$$x(x + 1)^2 f_6(x) - (x^2 - 1)^2 f(x) = (\alpha - 4)x^2 + 2x + (n - 2\alpha - 1). \quad (7)$$

Then from (7) we have

$$\begin{aligned} -(\rho^2 - 1)^2 f(\rho) &= (\alpha - 4)\rho^2 + 2\rho + (n - 2\alpha - 1) \\ &> (\alpha - 4)(\alpha + 1) + (n - 2\alpha - 1) \\ &= \alpha^2 - 5\alpha - 5 > 0. \end{aligned}$$

Thus  $f(\rho) < 0$ , then the largest root of equation  $f(x) = 0$  is larger than  $\rho$ , i.e.,  $\rho(M(n, \alpha)) > \rho(M_6(n, \alpha))$ .  $\square$

Denote by  $\mathcal{B}(n, \alpha, \alpha - 1, 3)$  the set of the graphs  $G$  in  $\mathcal{B}(n, \alpha, \alpha - 1)$  with  $|V'(G)| = 3$ .

**Lemma 4.10.** *Let  $G$  be a graph in  $\mathcal{B}(n, \alpha, \alpha - 1, 3)$ . Then  $\rho(G) < \rho(M(n, \alpha))$ .*

*Proof.* Let  $G^*$  be a graph with maximal spectral radius in  $\mathcal{B}(n, \alpha, \alpha - 1, 3)$ . First suppose that  $G^*$  is in  $\mathcal{B}_1(n)$ . Then  $\widehat{G^*} = B(3, \ell, q)$ . By using the similar arguments as the proofs of Lemma 4.3 we may deduce that  $\ell \leq 2$  and  $q = 3$ . Furthermore we have  $G^* \in \{M_4(n, \alpha), M_5(n, \alpha)\}$ . Combining Lemma 4.9 we have

$$\rho(G) \leq \rho(G^*) = \max\{\rho(M_4(n, \alpha)), \rho(M_5(n, \alpha))\} < \rho(M(n, \alpha)).$$

Now suppose that  $G^*$  is in  $\mathcal{B}_2(n)$ . Then we have  $G^* = M_6(n, \alpha)$ . By Lemma 4.9 we have

$$\rho(G) \leq \rho(G^*) = \rho(M_6(n, \alpha)) < \rho(M(n, \alpha)).$$

Thus we have  $\rho(G) < \rho(M(n, \alpha))$  for any graph  $G$  in  $\mathcal{B}(n, \alpha, \alpha - 1, 3)$ .  $\square$

Combining the results of Lemmas 4.6, 4.8 and 4.10 we have the following result.

**Theorem 4.3.** *Let  $G$  be any graph in  $\mathcal{B}(n, \alpha, \alpha - 1)$ . Then  $\rho(G) < \rho(M(n, \alpha))$ .*

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